

beta-Aminobutyric acid
541-48-0 | DTXSID4040975

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.12 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.91e-01

Confidence level: 8.38e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>beta-Aminobutyric acid</div> <div>Measured: 9.70</div> <div>Predicted: 9.12</div>	<div>Image not found</div> <div>4-Aminobutanoic acid</div> <div>Measured: 12.6</div> <div>Predicted: 9.58</div>	<div>Image not found</div> <div>5-Aminovaleric acid</div> <div>Measured: 8.54</div> <div>Predicted: 8.01</div>
<div>Image not found</div> <div>beta-Alanine</div> <div>Measured: 6.12</div> <div>Predicted: 7.73</div>	<div>Image not found</div> <div>6-Aminocaproic acid</div> <div>Measured: 3.85</div> <div>Predicted: 4.69</div>	